=> b reg;d que sta 115

FILE 'REGISTRY' ENTERED AT 17:40:51 ON 19 SEP 2007

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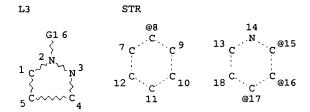
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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting ${\tt SmartSELECT}$ searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

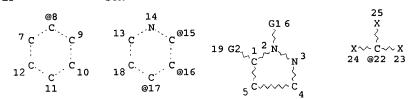
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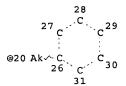


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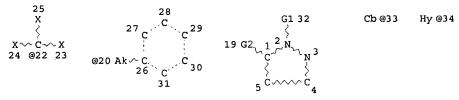




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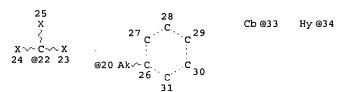
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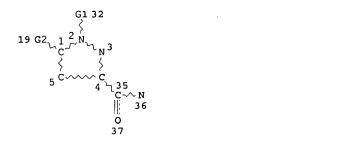
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NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

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CONNECT IS E2 RC AT 33

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 33

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DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M1-X5 C AT 20

ECOUNT IS E6 C AT 33

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NUMBER OF NODES IS 23

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GRAPH ATTRIBUTES:

RSPEC 2

NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE

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100.0% PROCESSED 4491 ITERATIONS

144 ANSWERS

SEARCH TIME: 00.00.01

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L24 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 2006:325402 HCAPLUS

DN 145:103666

TI Preparation of pyrazoles as cyclooxygenase inhibitors

PA Fujisawa Pharmaceutical Co., Ltd., Japan

SO Aust. Pat. Appl., 68 pp.

CODEN: AUXXCM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PΙ	AU2004200420	A1	20040930	2004AU-0200420	20040206 <
PRAI	2003AU-0901100	Α	20030311	<	

OS MARPAT 145:103666

GT

AB The title compds. I [R1 = halo, CN, alkylcarbonyl, etc.; R2 = halo, CN, alkyl, etc.; R3 = H, alkyl; R4 = halo, CN, NO2, alkyl, etc.; or R3 and R4 may form 2,3-dihydrofuryl; R5 = OH and R6 = H in case of single bond between carbon atoms to which R5 and R6 are attached; or R5 and R6 do not exist in case of double bond; Y = CH and Z = N, Y = N and Z = CH, or Y = N and Z = N], useful for treating and/or preventing inflammatory conditions, various pains, collagen disease, autoimmune diseases, various immunity diseases, thrombosis, cancer or neurodegenerative diseases, were prepared Thus, treating a solution of 5-amino-2-methoxypyridine in 1N HCl with sodium nitrite and with tin (II) chloride dihydrate followed by addition of 4-(4,4-difluoro-3-oxobutanoyl)benzonitrile and acetic acid afforded 32% 5-(4-cyanophenyl)-3-difluoromethyl-1-(6-methoxy-3-pyridyl)-1H-pyrazole which showed IC50 of <0.01 µM against COX-1. Pharmaceutical composition comprising the compound I is disclosed.

IT 741286-77-1P 741286-88-4P 896133-10-1P

Т

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of pyrazoles as cyclooxygenase inhibitors)

RN 741286-77-1 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 1-(6-methoxy-3-pyridinyl)-5-(4methylphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 741286-88-4 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-(4-methoxyphenyl)-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 896133-10-1 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-(4-cyanophenyl)-1-(6-methoxy-3-pyridinyl)-, ethyl ester (CA INDEX NAME)

IT 896133-22-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrazoles as cyclooxygenase inhibitors)

RN 896133-22-5 HCAPLUS

CN 1H-Pyrazole-3-methanol, 1-(6-methoxy-3-pyridinyl)- α , α -dimethyl-5-(4-methylphenyl)- (CA INDEX NAME)

L24 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:612279 HCAPLUS

DN 143:133365

Preparation of pyrazole carboxamide derivatives as platelet aggregation inhibitors for treatment of ischemia

IN Kanaya, Naoaki; Ishiyama, Takashi; Muto, Ryo; Ochiai, Yuichi; Watanabe, Toshiyuki; Kuru, Noriko

PA Daiichi Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 329 pp.

CODEN: PIXXD2
DT Patent

LA Japanese

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FAN.CNT 1
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     2004WO-JP19582
os
     MARPAT 143:133365
GI
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AB Title compds. represented by the formula I [wherein Ar1, Ar2 = independently (un) substituted (hetero) aryl; R1 = alkyl, alkoxycarbonyl, acyl, etc.; R2 = H, alkyl; and their salts or solvates thereof] were prepared as platelet aggregation inhibitors. For example, II was given in a multi-step synthesis starting from 5-amino-2-methoxypyridine. I showed inhibition of platelet aggregation, but not for COX-1 and COX-2. Thus, I and their pharmaceutical compns. are useful prepared as platelet aggregation inhibitors for the treatment of ischemia.

IT 741286-83-9P 741287-84-3P 858598-00-2P

858598-10-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrazole carboxamide derivs. as platelet aggregation inhibitors for treatment of ischemia)

RN 741286-83-9 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 1-(6-methoxy-3-pyridinyl)-5-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ \parallel & & & \\ \hline & N & & \\ \hline & N & & \\ \hline & N & & & \\$$

741287-84-3 HCAPLUS

RN

CN 1H-Pyrazole-3-carboxylic acid, 1-(5-methoxy-2-pyridinyl)-5-phenyl-, ethyl

ester (9CI) (CA INDEX NAME)

858598-00-2 HCAPLUS RN

1H-Pyrazole-3-carboxylic acid, 5-[3-(dimethylamino)phenyl]-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 858598-10-4 HCAPLUS

1H-Pyrazole-3-carboxylic acid, 5-[4-(dimethylamino)phenyl]-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME) CN

THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 14 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:612278 HCAPLUS

DN 143:133364

ΤI Preparation of pyrazole carboxamide derivatives as platelet aggregation inhibitors for treatment of ischemia

Horino, Haruhiko; Kanaya, Naoaki IN

Daiichi Pharmaceutical Co., Ltd., Japan PA

PCT Int. Appl., 60 pp. so

CODEN: PIXXD2

DTPatent

	CNT 1	E																
	PATENT	NO.			KIN	D	DATE			APPL	ICAT	ION :	NO.		D	ATE		
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10 / 552064

NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, RO, SE, SI, MR, NE, SN, TD, TG 20070405 20031226 <--JP2007084437 2003JP-0433974 Α PRAI 2003JP-0433974 Α 20031226 <--MARPAT 143:133364 OS GI

AB Title compds. represented by the formula I [wherein Ar1, Ar2 = independently (un) substituted (hetero)aryl; R1, R2 = independently H or alkyl; R3 = H or (un) substituted alkyl; R4 = (un) substituted alkyl, amino, alkoxy, carbamoyl, heterocyclyl; n = 0 or 1; and their salts or solvates thereof] were prepared as platelet aggregation inhibitors. For example, II was given in a multi-step synthesis starting from 5-amino-2-methoxypyridine. I showed inhibition of platelet aggregation, but not for COX-1 and COX-2. Thus, I and their pharmaceutical compns. are useful as platelet aggregation inhibitors for the treatment of ischemia.

741286-83-9P 741287-25-2P 858520-67-9P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrazole carboxamide derivs. as platelet aggregation inhibitors for treatment of ischemia)

RN 741286-83-9 HCAPLUS

IT

RN 741287-25-2 HCAPLUS CN 1H-Pyrazole-3-methanol, 1-(6-methoxy-3-pyridin

1H-Pyrazole-3-methanol, 1-(6-methoxy-3-pyridinyl)-5-phenyl- (9CI) (CA INDEX NAME)

RN 858520-67-9 HCAPLUS CN 1H-Pyrazole-3-methanol, 1-(6-methoxy-3-pyridinyl)- α -methyl-5-phenyl-(9CI) (CA INDEX NAME)

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN
L24
     2004:675738 HCAPLUS
AN
DN
     141:207201
ΤI
     Preparation of pyrazole derivatives as antiplatelet aggregation agents for
     the treatment of ischemic diseases
     Kanaya, Naoaki; Ishihara, Hiroaki; Kimura, Youichi; Ishiyama, Takashi;
IN
     Ochiai, Yuichi
PA
     Daiichi Pharmaceutical Co., Ltd., Japan
so
     PCT Int. Appl., 383 pp.
     CODEN: PIXXD2
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FAN.CNT 1
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                                                                    DATE
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$$\begin{array}{c}
R^{2} \\
R^{3}
\end{array}$$

Title compds. I [Arl = aromatic heterocycle; Ar2 = aromatic heterocycle, etc.; AB R1 = II; A = cycle containing N, S, O; X = carbonyl, etc.; R3 = H, halo, etc.; R2 = H, halo, etc.] were prepared For example, N-(3-Dimethylaminopropyl)-N'ethylcarbodiimide HCl mediated acylation of N-cyclopropylpiperazine hydrochloride with 1-(6-methoxy-3-pyridyl)-5-(2-pyridyl)pyrazole-3carboxylic acid, e.g., prepared from 2-acetylpyridine in 3 steps, afforded compound I [Ar1 = 2-methoxypyridin-5-yl; Ar2 = 2-pyridyl; R1 = 1-cyclopropylpiperazine-4-carbonyl; R2 = H] in 83% yield. In antiplatelet activity assays, the IC50 value of compound I [Ar1 = 2-methoxypyridin-5-yl; Ar2 = 2-pyridyl; R1 = 1-cyclopropylpiperazine-4-carbonyl; R2 = H] was 0.035 μM . Of note, compds. I inhibited neither COX-1 nor COX-2. Compds. I are claimed useful for the treatment of ischemic diseases. IT 741286-30-6P 741286-33-9P 741286-43-1P 741286-47-5P 741286-53-3P 741286-77-1P 741286-81-7P 741286-83-9P 741286-88-4P

RN 741286-33-9 HCAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 5-(4-ethylphenyl)-1-(6-methoxy-3-pyridinyl), ethyl ester (9CI) (CA INDEX NAME)

RN 741286-43-1 HCAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-(6-methoxy-3-pyridinyl)-5-(2-methylphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 741286-47-5 HCAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 5-(3-fluorophenyl)-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN

741286-53-3 HCAPLUS
1H-Pyrazole-3-carboxylic acid, 1-(6-methoxy-3-pyridinyl)-5-[4-(phenylmethoxy)phenyl]-, ethyl ester (9CI) (CA INDEX NAME) CN

RN

741286-77-1 HCAPLUS
1H-Pyrazole-3-carboxylic acid, 1-(6-methoxy-3-pyridinyl)-5-(4-methylphenyl)-, ethyl ester (9CI) (CA INDEX NAME) CN

RN

741286-81-7 HCAPLUS
1H-Pyrazole-3-carboxylic acid, 5-(2-fluorophenyl)-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME) CN

RN

741286-83-9 HCAPLUS

1H-Pyrazole-3-carboxylic acid, 1-(6-methoxy-3-pyridinyl)-5-phenyl-, ethyl CN

ester (9CI) (CA INDEX NAME)

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CN 1H-Pyrazole-3-carboxylic acid, 5-(4-methoxyphenyl)-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 741286-91-9 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-(3-methoxyphenyl)-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

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RN 741286-95-3 HCAPLUS

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RN 741287-25-2 HCAPLUS CN 1H-Pyrazole-3-methanol, 1-(6-methoxy-3-pyridinyl)-5-phenyl- (9CI) (CA INDEX NAME)

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CN 1H-Pyrazole-3-carboxylic acid, 5-(4-fluorophenyl)-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 741287-84-3 HCAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-(5-methoxy-2-pyridinyl)-5-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

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RN 741291-47-4 HCAPLUS
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MARPAT 141:54327

OS GI

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TI
IN
     Shirai, Fumiyuki; Azami, Hidenori; Kayakiri, Natsuko; Okumura, Kazuo;
     Nakamura, Katsuya
PA
     Fujisawa Pharmaceutical Co., Ltd., Japan
SO
     PCT Int. Appl., 436 pp.
     CODEN: PIXXD2
DT
     Patent
T.A
     English
FAN.CNT 3
     PATENT NO.
                          KIND
                                DATE
                                             APPLICATION NO.
                                                                    DATE
ΡI
                                 20040617
                                             2003WO-JP14489
                                                                    20031114 <--
     WO2004050632
                          A1
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG,
                         RO, RU, SC,
                                     SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR,
             PH, PL, PT,
             TT, TZ, UA,
                         UG, US, UZ,
                                     VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
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             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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                                                                    20031114 <--
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     EP---1567503
                          A1
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     2003AU-0902015
                          Α
                                 20030429
                                           <--
     2003WO-JP14489
                                 20031114 <--
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$$R^4-z-x$$

The compds. [I; R1 = H, alkyl; R2 = alkyl, haloalkyl, hydroxyalkyl, etc.; R3 = alkoxy, halo, CN, etc.; R4 = H, CN, OH, etc.; X = 0, S, SO, SO2; Y = CH, N; Z = alkylene, alkenylene; m = 0-1], were prepared E.g., a 3-step synthesis of 4-[3-isopropyl-1-(4-methoxyphenyl)-1H-pyrazol-5-yl]phenol, was given. The compds. I have an inhibiting activity against COX, particularly a selective inhibiting activity against COX-1 (data for representative compds. I is given). The pharmaceutical composition comprising the compound I is claimed.

IT 705933-46-6P
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of pyrazole derivs. useful as COX-1 inhibitors)

RN 705933-46-6 HCAPLUS
CN Carbamic acid, [2-[4-[3-(1-hydroxy-1-methylethyl)-1-(6-methoxy-3-pyridinyl)-1H-pyrazol-5-yl]phenoxy]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 705935-79-1 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-[4-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethoxy]phenyl]-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 705936-08-9 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-[4-(carboxymethoxy)phenyl]-1-(6-methoxy-3pyridinyl)-, 3-ethyl ester (9CI) (CA INDEX NAME)

RN 705936-11-4 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-[4-(2-hydroxyethoxy)phenyl]-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 705937-87-7 HCAPLUS

CN Carbamic acid, [[4-[3-(1-hydroxy-1-methylethyl)-1-(6-methoxy-3-pyridinyl)-1H-pyrazol-5-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 705938-84-7 HCAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 5-[4-(aminomethyl)phenyl]-1-(6-methoxy-3-pyridinyl)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

RN 705938-88-1 HCAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 5-[4-[[[(1,1-dimethylethoxy)carbonyl]amino]
 methyl]phenyl]-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX
 NAME)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN

I

AN 2004:493568 HCAPLUS

DN 141:54325

TI Preparation of pyrazole derivatives useful as COX-1 inhibitors

IN Shirai, Fumiyuki; Azami, Hidenori; Kayakiri, Natsuko; Okumura, Kazuo; Nakamura, Katsuya

PA Fujisawa Pharmaceutical Co., Ltd., Japan

SO U.S. Pat. Appl. Publ., 142 pp.

CODEN: USXXCO

DT Patent

LA English

1	FAN.	CNT 3				
		PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
1	PI	US2004116475	A1	20040617	2003US-0706999	20031114 <
		US7183306	B2	20070227		
		CN1717393	A	20060104	CN 2003-80104548	20031114 <
		US2007112037	A1	20070517	2006US-0610230	20061213 <
1	PRAI	2002AU-0953019	Α	20021202	<	
		2002AU-0953602	A	20021230	<	
		2003AU-0902015	A	20030429	<	
		2003US-0706999	A 3	20031114	<	
(os	MARPAT 141:54325				
•	T.					

The compds. [I; R1 = H, alkyl; R2 = alkyl, haloalkyl, hydroxyalkyl, etc.; R3 = alkoxy, halo, CN, etc.; R4 = H, CN, OH, etc.; X = 0, S, SO, SO2; Y = CH, N; Z = alkylene, alkenylene; m = 0-1], were prepared E.g., a 3-step synthesis of 4-[3-isopropyl-1-(4-methoxyphenyl)-1H-pyrazol-5-yl]phenol, was given. The compds. I have an inhibiting activity against COX, particularly a selective inhibiting activity against COX-1 (data for representative compds. I is given). The pharmaceutical composition comprising the compound I is claimed.

IT 705933-46-6P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of pyrazole derivs. useful as COX-1 inhibitors)

RN 705933-46-6 HCAPLUS

CN Carbamic acid, [2-[4-[3-(1-hydroxy-1-methylethyl)-1-(6-methoxy-3-pyridinyl)-1H-pyrazol-5-yl]phenoxy]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 705934-45-8P 705935-79-1P 705936-08-9P 705936-11-4P 705937-87-7P 705938-84-7P 705938-88-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrazole derivs. useful as COX-1 inhibitors)

RN 705934-45-8 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-[4-[2-(acetyloxy)ethyl]phenyl]-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 705936-08-9 HCAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 5-[4-(carboxymethoxy)phenyl]-1-(6-methoxy-3-pyridinyl)-, 3-ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} \\ & N \\ & O - CH_2 - CO_2H \\ & O \\ & O$$

RN 705936-11-4 HCAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 5-[4-(2-hydroxyethoxy)phenyl]-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 705937-87-7 HCAPLUS
CN Carbamic acid, [[4-[3-(1-hydroxy-1-methylethyl)-1-(6-methoxy-3-pyridinyl)1H-pyrazol-5-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 705938-84-7 HCAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 5-[4-(aminomethyl)phenyl]-1-(6-methoxy-3-pyridinyl)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

RN 705938-88-1 HCAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 5-[4-[[[(1,1-dimethylethoxy)carbonyl]amino]
 methyl]phenyl]-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX
 NAME)

RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 2003:279562 HCAPLUS

DN 138:304276

TI Preparation of pyrazoles as glycine transporter protein inhibitors for the treatment of neurodegenerative diseases

PA Merck Patent G.m.b.H., Germany; Yamanouchi Pharmaceutical Co.

SO Ger. Offen., 62 pp.

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CODEN: GWXXBX Patent
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LA German

DT

FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE DE--10149370 20030410 2001DE-1049370 20011006 <--PТ A1. 20030417 20020911 <--WO2003031435 **A1** 2002WO-EP10172 WO2003031435 20030515 **8**A W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, KG, KZ, MD, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, FI, FR, GB, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG AU2002342675 A1 20030422 2002AU-0342675 20020911 <--PRAI 2001DE-1049370 Α 20011006 2002WO-EP10172 W 20020911 <--MARPAT 138:304276 os GI

$$R^1$$
 X
 R^2
 R^3

II

ΙV

I

III

AB Title compds. I [X = CH, N; R1 = H, A, halo, etc.; R2 = Ph, p-chlorophenyl; R3, R4 = H, (CH2)nCO2R5, CHO, etc.; R5 = H, A; A = alkyl, alkenyl, alkoxyalkyl, etc.; n = 0-5] and their pharmaceutically acceptable salts were prepared For example, condensation of enamine II e.g., prepared from 1,1-dimethoxy-N,N-dimethylmethanamine and 2-fluoro-β-oxobenzenepropanoic acid Et ester, and aryl hydrazine III, e.g., prepared from 2-chloro-5-nitropyridine in 3-steps, provided pyrazole IV (no yield provided). In glycine transporter protein inhibition studies, approx. 71-examples of compds. I exhibited IC50 values ranging from 0.15 - 8.7 μM, e.g., the IC50 value of pyrazole IV = 2.5 μM. Compds. I are claimed useful for the treatment of schizophrenia, depression, dementia, etc.

IT 508219-76-9P, 5-(2-Fluorophenyl)-1-(6-phenylpyridin-3-yl)-1Hpyrazol-4-carboxylic acid ethyl ester
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; preparation of pyrazoles as glycine transporter protein inhibitors for the treatment of neurodegenerative diseases)

RN 508219-76-9 HCAPLUS

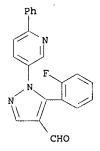
CN 1H-Pyrazole-4-carboxylic acid, 5-(2-fluorophenyl)-1-(6-phenyl-3-pyridinyl), ethyl ester (9CI) (CA INDEX NAME)

IT

RN

CN

508219-82-7
RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of pyrazoles as glycine transporter protein inhibitors for the treatment of neurodegenerative diseases)
508219-82-7 HCAPLUS
1H-Pyrazole-4-carboxaldehyde, 5-(2-fluorophenyl)-1-(6-phenyl-3-pyridinyl)-(9CI) (CA INDEX NAME)



L24 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 1987:423332 HCAPLUS

DN 107:23332

TI Cyanopyrazole derivatives as intermediates for herbicides and algicides.

IN Beck, James R.

PA Eli Lilly and Co., USA

SO U.S., 10 pp. Cont.-in-part of U.S. Ser. No. 549,111, abandoned.

CODEN: USXXAM

DT Patent English LA FAN. CNT 1

PATENT NO. KIND DATE Α 19861223 PΙ US---4631343

DATE APPLICATION NO. 19840913 <--1984US-0650160

PRAI 1983US-0549111 19831107 <--A2 CASREACT 107:23332; MARPAT 107:23332

GI

The title compds. [I; R1 = C5-6 cycloalkyl, 2-quinolinyl, (un) substituted AΒ Ph, 2-pyridinyl, 4-pyridinyl; R2 = C1-4 (halo)alkyl, (halo)alkoxy, halo] were prepared as intermediates for 5-cyano-1H-pyrazole-4-carboxamide herbicides (no data). 2-Hydrazinopyridine and EtOCH:C(CN)CO2Et were heated in HOAc to give pyridinylpyrazolecarboxylate II (R2 = EtO, R3 = NH2). This was chlorinated with NOCl and cyanated with NaCN to give II (R2 = EtO, R3 = cyano) which was heated with MeNH2 to give II (R2 = MeNH, R3 = cyano).

IT 98476-17-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as algicide and herbicide intermediate) 98476-17-6 HCAPLUS

RN

1H-Pyrazole-4-carboxylic acid, 1-(5-chloro-2-pyridinyl)-5-cyano-, ethyl ester (9CI) (CA INDEX NAME)

L24 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 1985:541948 HCAPLUS

103:141948 DN

Cyanopyrazole herbicides TI

Beck, James Richard IN

PA Eli Lilly and Co., USA

Brit. UK Pat. Appl., 28 pp.

CODEN: BAXXDU

דת Patent

LΑ English

FAN CNT 1

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	IL73418	Α	19880229	1984IL-0073418	19841104 <
	EP151867	A2	19850821	1984EP-0307629	19841105 <
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	EP151867	B1	19900110		
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	ZA8408666	Α	19860129	1984ZA-0008666	19841106 <

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PRAI 1983US-0549133
                           Α
                                 19841105 <--
     1984EP-0307629
                          Α
os
     CASREACT 103:141948; MARPAT 103:141948
GI
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AB Cyanopyrazoles I [R = alkyl, cycloalkyl, 2-quinolinyl, (un)substituted Ph, 2-pyridyl, 4-pyridyl; R1, R2 = H, alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy; NR1R2 = piperidino, morpholino, pyrrolidino; X = 0, S] (101 compds.) were prepared Thus, Me3CNHNH2.HCl was cyclocondensed with Me2NCH:C(COMe)CO2Et to give Et 5-methyl-1-tert-butyl-1H-pyrazole-4-carboxylate, which was brominated with NBS to give the 5-(bromomethyl) compound The latter compound, by the procedure described by H. B. Hass and M. L. Bender (1949), was converted to the 5-formyl compound, which was treated with H2NOH.HCl to give the oxime. The oxime was dehydrated with SOCl2 to give Et 5-cyano-1-tert-butyl-1H-pyrazole-4-carboxylate which was saponified to the carboxylic acid. The acid was treated with carbonyldiimidazole and MeNH2 to give I (R = Me3C, R1 = Me, R2 = H, X = O). I are useful both as preemergent and postemergent herbicides (no data).

IT 98476-17-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(amidation of)

RN 98476-17-6 HCAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(5-chloro-2-pyridinyl)-5-cyano-, ethyl ester (9CI) (CA INDEX NAME)

=> => b uspatall FILE 'USPATFULL' ENTERED AT 17:42:46 ON 19 SEP 2007 CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPATOLD' ENTERED AT 17:42:46 ON 19 SEP 2007 CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS) .

FILE 'USPAT2' ENTERED AT 17:42:46 ON 19 SEP 2007
CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

=> d bib abs hitstr 126 tot

US-20070112037

PΙ

A1 20070517

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ΑI
       2006US-000610230
                          A1 20061213 (11)
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       Division of Ser. No. 2003US-000706999, filed on 14 Nov 2003, GRANTED,
       Pat. No. US----7183306
PRAI
       2002AU-2002953019
                            20021202
       2002AU-2002953602
                            20021230
       2003AU-2003902015
                            20030429
דת
       Utility
       APPLICATION
FS
LREP
       OBLON, SPIVAK, MCCLELLAND, MAIER & NEUSTADT, P.C., 1940 DUKE STREET,
       ALEXANDRIA, VA, 22314, US
       Number of Claims: 12
CLMN
ECL
       Exemplary Claim: 1
DRWN
       No Drawings
LN.CNT 9883
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
       A compound of the formula (I):
                                          ##STR1## wherein
AB
R.sup.1 is hydrogen or lower alkyl;
R.sup.2 is lower alkyl, etc.;
R.sup.3 is lower alkoxy, etc.;
R.sup.4 is hydroxy, etc.; X is O, S, etc.; Y is CH or N; Z is lower alkylene or
       lower alkenylene; and m is 0 or 1; or salts thereof, which are useful as
       a medicament.
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 705939-67-9P
        (preparation of pyrazole derivs. useful as COX-1 inhibitors)
RN
     705939-67-9 USPATFULL
CN
     1H-Pyrazole-3-carboxylic acid, 5-(4-hydroxyphenyl)-1-(6-methoxy-3-
       pyridinyl) -, ethyl ester (9CI) (CA INDEX NAME)
L26 ANSWER 2 OF 6 USPATFULL on STN AN 2006:152244 USPATFULL
       Pyrazole derivative
TI
       Kanaya, Naoaki, Tokyo, JAPAN
IN
       Ishihara, Hiroaki, Tokyo, JAPAN
       Kimura, Youichi, Tokyo, JAPAN
       Ishiyama, Takashi, Tokyo, JAPAN
       Ochiai, Yuichi, Tokyo, JAPAN
DAIICHI PHARMACEUTICAL CO., LTD.,, Tokyo, JAPAN, 103-8234 (non-U.S.
PA
       corporation)
       US-20060128685
                            A1 20060615
PΙ
       2004US-000543915
                            A1 20040206 (10)
AΙ
       2004WO-JP0001259
                                20040206
                                20050729 PCT 371 date
PRAI
       2003JP-0000031639
                            20030207
       2003JP-000386515
                            20031117
DT
       Utility
FS
       APPLICATION
LREP
       OBLON, SPIVAK, MCCLELLAND, MAIER & NEUSTADT, P.C., 1940 DUKE STREET,
       ALEXANDRIA, VA, 22314, US
       Number of Claims: 19
CLMN
ECL
       Exemplary Claim: 1
DRWN
       No Drawings
LN.CNT 8901
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
       The present invention is directed to a strong platelet
AB
       aggregation-inhibiting agent which does not inhibit {\tt COX-1} or {\tt COX-2}.
       The present invention provides compounds represented by formula (I) or
       formula (II), salts of the compounds, and solvates of the compounds or
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the salts. Also provided are medicaments containing any of the compounds, salts, or solvates and preventive and/or therapeutic agents for ischemic diseases, containing any of the compounds, salts, or the solvates. ##STR1##

RN 741286-47-5 USPATFULL CN 1H-Pyrazole-3-carboxylic acid, 5-(3-fluorophenyl)-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 741286-81-7 USPATFULL CN 1H-Pyrazole-3-carboxylic acid, 5-(2-fluorophenyl)-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 741286-83-9 USPATFULL CN 1H-Pyrazole-3-carboxylic acid, 1-(6-methoxy-3-pyridinyl)-5-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 741286-88-4 USPATFULL CN 1H-Pyrazole-3-carboxylic acid, 5-(4-methoxyphenyl)-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 741286-91-9 USPATFULL CN 1H-Pyrazole-3-carboxylic acid, 5-(3-methoxyphenyl)-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 741286-93-1 USPATFULL CN 1H-Pyrazole-3-carboxylic acid, 5-(2-methoxyphenyl)-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 741287-78-5 USPATFULL CN 1H-Pyrazole-3-carboxylic acid, 5-(4-fluorophenyl)-1-(6-methoxy-3-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

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EtO-C N N OME
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IT 705939-67-9P

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L26 ANSWER 3 OF 6 USPATFULL on STN AN 2004:152253 USPATFULL
       Pyrazole derivatives
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       Shirai, Fumiyuki, Osaka, JAPAN
Azami, Hidenori, Osaka, JAPAN
IN
       Kayakiri, Natsuko, Osaka, JAPAN
       Okumura, Kazuo, Osaka, JAPAN
       Nakamura, Katsuya, Osaka, JAPAN
       FUJISAWA PHARMACEUTICAL CO., LTD., Osaka-shi, JAPAN (non-U.S.
PA
        corporation)
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B2 20070227
A1 20031114 (10)
ΡI
       US-20040116475
        US----7183306
ΑI
       2003US-000706999
                              20021202
PRAI
        2002AU-2002953019
        2002AU-2002953602
                              20021230
        2003AU-2003902015
                              20030429
        Utility
DT
FS
        APPLICATION
        OBLON, SPIVAK, MCCLELLAND, MAIER & NEUSTADT, P.C., 1940 DUKE STREET,
LREP
       ALEXANDRIA, VA, 22314
Number of Claims: 12
CLMN
ECL
        Exemplary Claim: 1
DRWN
       No Drawings
LN.CNT 9237
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
                                            ##STR1##
AΒ
       A compound of the formula (I):
        wherein R.sup.1 is hydrogen or lower alkyl;
       R.sup.2 is lower alkyl, etc.;
       R.sup.3 is lower alkoxy, etc.;
       R.sup.4 is hydroxy, etc.;
       X is O, S, etc.;
       Y is CH or N;
        Z is lower alkylene or lower alkenylene; and
        m is 0 or 1; or salts thereof, which are useful as a medicament.
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
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10 / 552064

(preparation of pyrazole derivs. useful as COX-1 inhibitors) RN 705939-67-9 USPATFULL 1H-Pyrazole-3-carboxylic acid, 5-(4-hydroxyphenyl)-1-(6-methoxy-3-CN pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

L26 ANSWER 4 OF 6 USPATFULL on STN AN 86:73304 USPATFULL Cyanopyrazole intermediates TI Beck, James R., Indianapolis, IN, United States IN Eli Lilly and Company, Indianapolis, IN, United States (U.S. PΑ corporation) ΡI US----4631343 19861223 1984US-000650160 19840913 (6) AΙ Continuation-in-part of Ser. No. 1983US-000549111, filed on 7 Nov 1983, RLT now abandoned DT Utility Granted FS Primary Examiner: Schwartz, Richard A.; Assistant Examiner: Briscoe, EXNAM Page, Kathleen R. S., Jones, Joseph A. LREP Number of Claims: 15 CT.MN ECL Exemplary Claim: 1 DRWN No Drawings LN.CNT 769 CAS INDEXING IS AVAILABLE FOR THIS PATENT. 5-Cyano-1-substituted-1H-pyrazole-4-carboxylic acids and esters useful AB

as intermediates to the corresponding 4-carboxyamide derivatives having herbicidal and algicidal activity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 98476-17-6P

(preparation of, as algicide and herbicide intermediate)

98476-17-6 USPATFULL RN

1H-Pyrazole-4-carboxylic acid, 1-(5-chloro-2-pyridinyl)-5-cyano-, ethyl CN ester (9CI) (CA INDEX NAME)

```
L26 ANSWER 5 OF 6 USPATFULL on STN AN 86:29482 USPATFULL
TI
         Herbicidal and algicidal 1-aryl-5-cyano-1H-pyrazole-4-carboxamides
        Beck, James R., Indianapolis, IN, United States
Eli Lilly and Company, Indianapolis, IN, United States (U.S.
IN
PA
         corporation)
PI
         US----4589905
                                      19860520
         1984US-000650132
                                      19840913 (6)
ΑI
         Continuation-in-part of Ser. No. 1983US-000549133, filed on 7 Nov 1983,
RLT
         now abandoned
\mathbf{DT}
         Utility
FS
         Granted
```

EXNAM Primary Examiner: Schwartz, Richard A.; Assistant Examiner: Briscoe, LREP Page, Kathleen R. S., Barclay, Bruce J., Whale, Arthur R. Number of Claims: 45 CLMN ECL Exemplary Claim: 1,33 DRWN No Drawings LN.CNT 2614 CAS INDEXING IS AVAILABLE FOR THIS PATENT. The present invention is directed to compounds of the formula ##STR1## wherein R.sup.1 is C.sub.1 -C.sub.6 alkyl, C.sub.5 -C.sub.6 cycloalkyl, ##STR2## each of R.sup.2 and R.sup.3 is taken separately and is independently hydrogen, C.sub.1 -C.sub.4 alkyl, C.sub.3 -C.sub.4 alkenyl, C.sub.3 -C.sub.4 alkynyl, C.sub.3 -C.sub.4 cycloalkyl or C.sub.1 -C.sub.3 alkoxy, or R.sup.2 and R.sup.3 are taken together with the nitrogen atom to which they are attached and form piperidine, morpholine or pyrrolidine; each R.sup.4 independently is halogen, C.sub.1 -C.sub.4 alkyl, C.sub.1 -Cphd 4 alkoxy, C.sub.1 -C.sub.4 haloalkyl, C.sub.1 -C.sub.4 haloalkoxy or cvano: X is 0 or S; and m is 0-3; with the provisos that when R.sup.4 is C.sub.1 -C.sub.4 alkyl, that substituent exists at other than the 2 or 6 position of the phenyl ring; and when R.sup.2 is C.sub.1 -C.sub.3 alkoxy, R.sup.3 is other than C.sub.1 -C.sub.3 alkoxy. These compounds exhibit activity as terrestrial herbicides, aquatic herbicides, and aquatic algicides. CAS INDEXING IS AVAILABLE FOR THIS PATENT. IT 98476-17-6 (amidation of) 98476-17-6 USPATFULL RN 1H-Pyrazole-4-carboxylic acid, 1-(5-chloro-2-pyridinyl)-5-cyano-, ethyl CN ester (9CI) (CA INDEX NAME) L26 ANSWER 6 OF 6 USPAT2 on STN 2004:152253 USPAT2 AN TT Pyrazole derivatives Shirai, Fumiyuki, Osaka, JAPAN IN Azami, Hidenori, Osaka, JAPAN Kayakiri, Natsuko, Osaka, JAPAN Okumura, Kazuo, Osaka, JAPAN Nakamura, Katsuya, Osaka, JAPAN PA Astellas Pharma Inc., Tokyo, JAPAN (non-U.S. corporation) US----7183306 B2 20070227 PΙ 2003US-000706999 20031114 (10) ΑI PRAI 2002AU-2002953019 20021202 2002AU-2002953602 20021230

2003AU-2003902015 20030429 DT Utility GRANTED FS EXNAM Primary Examiner: Morris, Patricia L. Oblon, Spivak, McClelland, Maier & Neustadt, P.C. LREP CLMN Number of Claims: 6 ECL Exemplary Claim: 1 DRWN No Drawings LN.CNT 9563 CAS INDEXING IS AVAILABLE FOR THIS PATENT.

```
AB
       A compound of the formula (I):
                   wherein R.sup.1 is hydrogen or lower alkyl;
        ##STR1##
R.sup.2 is lower alkyl, etc.;
R.sup.3 is lower alkoxy, etc.;
R.sup.4 is hydroxy, etc.;
X is O, S, etc.;
Y is CH or N;
Z is lower alkylene or lower alkenylene; and
m is 0 or 1; or salts thereof, which are useful as a medicament.
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 705939-67-9P
         (preparation of pyrazole derivs. useful as COX-1 inhibitors)
     705939-67-9 USPAT2
RN
     1H-Pyrazole-3-carboxylic acid, 5-(4-hydroxyphenyl)-1-(6-methoxy-3-
CN
       pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)
                         OMe
=> d his
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L2
                ACT J064C1D/A
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L3
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L4
    (
                 STR
L5
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L7
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    (
L8
L9
                 STR
           2389) SEA FILE=REGISTRY SUB=L8 SSS FUL L9
L10 (
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L13
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L14
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L16
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L17
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174 SEA L17 0 L15 AND L18

L18

L19

10 / 552064

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L23	12 L22 AND (C19H19N3O4 OR C18H16FN3O3 OR C12H9CLN4O2 OR C18H17N3O3
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1124	5 125 AND 121
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L25	6 L24
L26	6 L23
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L27	0 L23
	FILE 'USPATFULL, USPATOLD, USPAT2' ENTERED AT 17:42:46 ON 19 SEP 2007
	FIDE OSFAIFOLD, OSFAIOLD, OSFAIZ ENIERED AT 17:42.40 ON 19 SEF 2007
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